

# STN Process Search - Cas react

10/537,389

07/20/2007,

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\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS 1 Web Page for STN Seminar Schedule - N. America  
NEWS 2 MAR 15 WPIDS/WPIX enhanced with new FRAGHITSTR display format  
NEWS 3 MAR 16 CASREACT coverage extended  
NEWS 4 MAR 20 MARPAT now updated daily  
NEWS 5 MAR 22 LWPI reloaded  
NEWS 6 MAR 30 RDISCLOSURE reloaded with enhancements  
NEWS 7 APR 02 JICST-EPLUS removed from database clusters and STN  
NEWS 8 APR 30 GENBANK reloaded and enhanced with Genome Project ID field  
NEWS 9 APR 30 CHEMCATS enhanced with 1.2 million new records  
NEWS 10 APR 30 CA/Caplus enhanced with 1870-1889 U.S. patent records  
NEWS 11 APR 30 INPADOC replaced by INPADOCDB on STN  
NEWS 12 MAY 01 New CAS web site launched  
NEWS 13 MAY 08 CA/Caplus Indian patent publication number format defined  
NEWS 14 MAY 14 RDISCLOSURE on STN Easy enhanced with new search and display fields.  
NEWS 15 MAY 21 BIOSIS reloaded and enhanced with archival data  
NEWS 16 MAY 21 TOXCENTER enhanced with BIOSIS reload  
NEWS 17 MAY 21 CA/Caplus enhanced with additional kind codes for German patents  
NEWS 18 MAY 22 CA/Caplus enhanced with IPC reclassification in Japanese patents  
NEWS 19 JUN 27 CA/Caplus enhanced with pre-1967 CAS Registry Numbers  
NEWS 20 JUN 29 STN Viewer now available  
NEWS 21 JUN 29 STN Express, Version 8.2, now available  
NEWS 22 JUL 02 LEMBASE coverage updated  
NEWS 23 JUL 02 LMEDLINE coverage updated  
NEWS 24 JUL 02 SCISEARCH enhanced with complete author names  
NEWS 25 JUL 02 CHEMCATS accession numbers revised  
NEWS 26 JUL 02 CA/Caplus enhanced with utility model patents from China  
NEWS 27 JUL 16 Caplus enhanced with French and German abstracts  
NEWS 28 JUL 18 CA/Caplus patent coverage enhanced

NEWS EXPRESS 29 JUNE 2007: CURRENT WINDOWS VERSION IS V8.2,  
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),  
AND CURRENT DISCOVER FILE IS DATED 05 JULY 2007.

NEWS HOURS STN Operating Hours Plus Help Desk Availability

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NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 16:00:56 ON 20 JUL 2007

=> fil casreact

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'CASREACT' ENTERED AT 16:01:07 ON 20 JUL 2007

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FILE CONTENT:1840 - 14 Jul 2007 VOL 147 ISS 4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

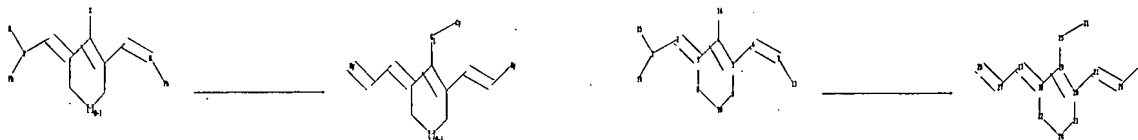
\*\*\*\*\*  
\*  
\* CASREACT now has more than 12 million reactions \*  
\*  
\*\*\*\*\*

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>

Uploading C:\Program Files\Stnexp\Queries\10537389\1.str



chain nodes :

1 2 6 7 13 14 15 16 17 21 25 26 27 28 29 31

ring nodes :

3 4 5 8 9 10 18 19 20 22 23 24

chain bonds :

1-2 1-14 1-15 2-3 4-16 5-6 6-7 7-13 17-18 17-27 19-25 20-21 21-26  
25-31 26-29 27-28

ring bonds :

3-4 3-8 4-5 5-9 8-10 9-10 18-19 18-22 19-20 20-23 22-24 23-24

exact/norm bonds :

1-2 3-4 3-8 4-5 5-9 6-7 8-10 9-10 18-19 18-22 19-20 19-25 20-23 22-24  
23-24 25-31 26-29 27-28

exact bonds :

1-14 1-15 2-3 4-16 5-6 7-13 17-18 17-27 20-21 21-26

G1:O,S,N,Se

Match level :

1:CLASS 2:CLASS 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:Atom 9:Atom 10:Atom  
13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:Atom 19:Atom 20:Atom  
21:CLASS 22:Atom 23:Atom 24:Atom 25:CLASS 26:CLASS 27:CLASS 28:Atom 29:Atom  
31:Atom

Element Count :

Node 28: Limited  
N,N1-2

Node 29: Limited  
N,N1-2

L1        STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1                STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 16:01:27 FILE 'CASREACT'

SCREENING COMPLETE -            27 REACTIONS TO VERIFY FROM            3 DOCUMENTS

100.0% DONE            27 VERIFIED            0 HIT RXNS            0 DOCS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:    ONLINE    \*\*COMPLETE\*\* ✓  
                                      BATCH    \*\*COMPLETE\*\* ✓

PROJECTED VERIFICATIONS:            229 TO            851

PROJECTED ANSWERS:            0 TO            0

L2            0 SEA SSS SAM L1 (            0 REACTIONS)

=> s l1 full ✓

FULL SEARCH INITIATED 16:01:35 FILE 'CASREACT'

SCREENING COMPLETE ✓            192 REACTIONS TO VERIFY FROM            31 DOCUMENTS

100.0% DONE ✓            192 VERIFIED            33 HIT RXNS ✓            5 DOCS ✓

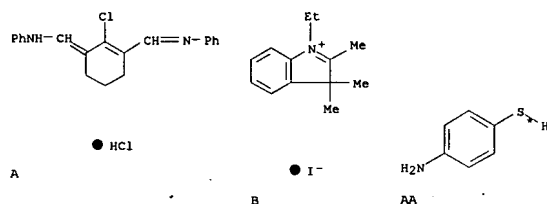
SEARCH TIME: 00.00.01

L3            5 SEA SSS FUL L1 (            33 REACTIONS)

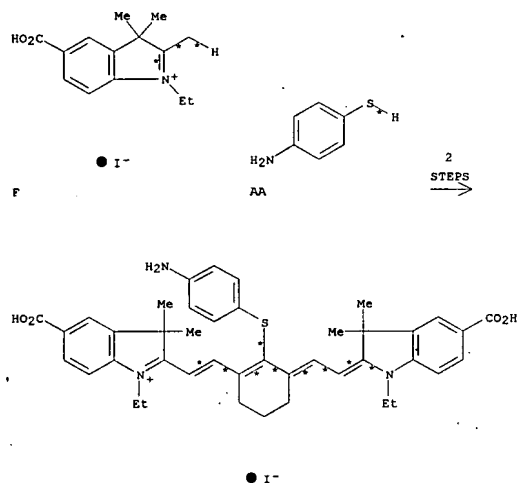
=> d ibib abs hit 1-5

L3 ANSWER 1 OF 5 CASREACT COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 145168977 CASREACT  
 TITLE: Synthesis and spectroscopic characterization of heptamethine cyanine NIR dyes for their use in optochemical sensors  
 AUTHOR(S): Encinas, Cristina; Miltsov, Serguei; Otazo, Elena; Rivera, Laia; Puyol, Mar; Alonso, Julian  
 CORPORATE SOURCE: Sensors & Biosensors Group, Analytical Chemistry, Autonomous University of Barcelona, Bellaterra, 08193, Spain  
 SOURCE: Dyes and Pigments (2005), Volume Date 2006, 71(1), 28-36  
 CODEN: DYPIDX; ISSN: 0143-7208  
 PUBLISHER: Elsevier Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB A set of near-IR absorbing tricarboyanine dyes has been synthesized and characterized for their future application as chromophores in optochem. sensors. Their absorption maxima are localized in the near-IR region, where matrix interferences are minimal and the use of suitable and inexpensive optical communication components gives great advantages. The acid form of the synthesized dyes in pure ethanol spans the region from 675 to 815 nm and the molar absorptivities are up to  $3.3 \times 10^5$  L/mol cm. The calculated pKa values in ethanol lie between 11.4 and more than 13.  
 The effect of the introduction of substituents on the pKa values and on the spectroscopic characteristics of the dyes is also discussed. Moreover, pH-sensitive aggregation processes have been observed in aqueous solution  
 REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(15) OF 18 COMPOSED OF RX(1), RX(11)  
 RX(15) A + B + AA ==> AB



L3 ANSWER 1 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



AC  
 YIELD 42%

RX(2) RCT A 63857-00-1, F 126442-85-1  
 RGT D 127-09-3 AcONa  
 PRO G 900807-92-3  
 SOL 64-17-5 EtOH  
 CON SUBSTAGE(1) 30 minutes, reflux  
 SUBSTAGE(2) overnight, -10 deg C  
 NTE acid-base equilibrium studied  
 RX(12) RCT G 900807-92-3, AA 1193-02-8  
 PRO AC 900807-97-8  
 NTE no experimental detail, acid-base equilibrium studied

RX(18) OF 18 COMPOSED OF RX(7), RX(13)  
 RX(18) A + 2 P + AA ==> AD

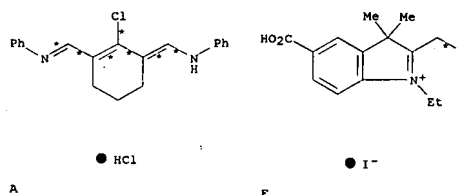
L3 ANSWER 1 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

2  
 STEPS  
 →

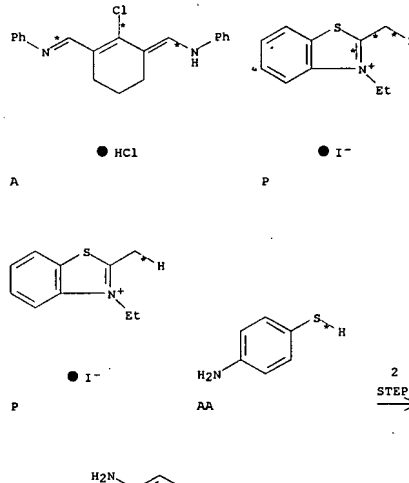
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(1) RCT A 63857-00-1, B 14134-81-7  
 RGT D 127-09-3 AcONa  
 PRO C 124591-86-2  
 SOL 64-17-5 EtOH  
 CON SUBSTAGE(1) 30 minutes, reflux  
 SUBSTAGE(2) overnight, -10 deg C  
 NTE acid-base equilibrium studied  
 RX(11) RCT C 124591-86-2, AA 1193-02-8  
 PRO AB 264915-22-2  
 NTE no experimental detail, acid-base equilibrium studied

RX(16) OF 18 COMPOSED OF RX(2), RX(12)  
 RX(16) A + 2 F + AA ==> AC



L3 ANSWER 1 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



AD  
 YIELD 45%

RX(7) RCT A 63857-00-1, P 3119-93-5  
 RGT D 127-09-3 AcONa  
 PRO Q 65303-15-3  
 SOL 64-17-5 EtOH

L3	ANSWER 1	OF 5	CASREACT	COPYRIGHT 2007 ACS on STN	(Continued)
	CON	SUBSTAGE(1)	30 minutes, reflux		
		SUBSTAGE(2)	overnight, -10 deg C		
	NTE	acid-base equilibrium	studied		
RX(13)	RCT	Q 65303-15-3,	AA 1193-02-8		
	PRO	AD 900807-98-9			
	NTE	no experimental detail,	acid-base equilibrium	studied	

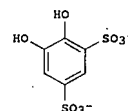
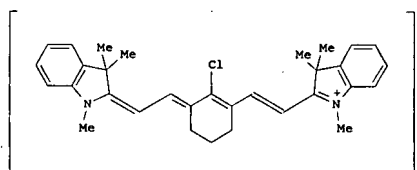
L3 ANSWER 2 OF 5 CASREACT COPYRIGHT 2007 ACS ON STN  
ACCESSION NUMBER: 142:483447 CASREACT  
TITLE: Process for the preparation of infrared absorbing  
cyanine dyes with polysulfonate anions  
INVENTOR(S): Tao, Ting; Kottmar, Eduard; Beckley, Scott A.  
PATENT ASSIGNEE(S): USA  
SOURCE: U.S. Pat. App. Publ., 15 pp.  
DOCUMENT TYPE: CODEN: USXXCO  
LANGUAGE: Patent  
FAMILY ACC. NUM. COUNT: English ✓  
PATENT INFORMATION: 1

Inventors

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005113546	A1	20050526	US 2003-722257	20031125
US 7132550	B2	20061107		
EP 1539968	A2	20050601	EP 2004-27416	20041118
R: DE, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, HR, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, IE, IS, YU				
JP 2005163039	A	20050623	JP 2004-340997	20041125
			US 2003-722257	20031125

PRIORITY APPLN. INFO.:  
FI

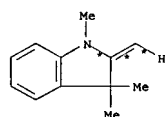
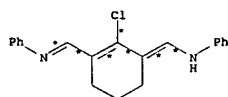
11/25/03



AB A convenient and economical method for preparing IR absorbing cyanine dyes

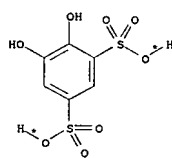
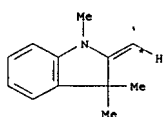
L3 ANSWER 2 OF 5 CASREACT COPYRIGHT 2007 ACS ON STN (Continued)  
is useful in lithog. printing plate precursors is disclosed. The reaction  
generally carried out by condensation of a heterocyclic base contg. an  
activated methylene group and an unsatd. bisaldehyde or its equiv. in a  
solvent or solvent mixt. at about 20-150°. All the reactions  
in necessary for prodn. of the IR absorbing cyanine dye may be carried out  
one reaction vessel without isolating any intermediate products. Thus,  
2-chloro-1-formyl-3-hydroxymethylcyclohexene was reacted with  
1,3,3-trimethyl-2-methyleneindoline (Fisher's base) to give a dark-green  
solin. which was then added to a soln. contg. disodium 4,5-dihydroxy-1,3-  
benzenedisulfonate to give a ppt. of an IR absorbing cyanine dye (I).  
REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS  
FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE

RX(7) OF 14      ...G + 2 J + P + K ==> O

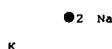


**G**

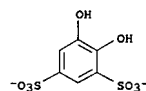
J



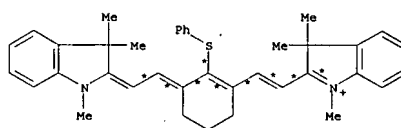
1



L3 ANSWER 2 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



O: CM 1



O: CM 2

RX(7) RCT G 63857-00-1. J 118-12-7

```
STAGE(1)
  SOL  64-17-5 ETOH
  CON  SUBSTAGE(1) 4 hours, 70 deg C
       SUBSTAGE(2) 70 deg C -> room temperature
```

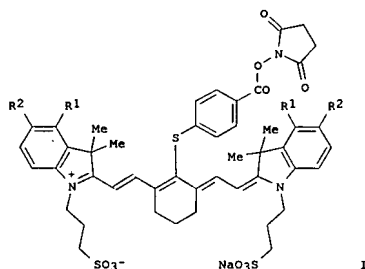
STAGE (2)  
RCT P 108-98-5  
RGT R 1310-73-2 NaOH  
SOL 64-17-5 EtOH  
CON 15 hours, room temperature

STAGE (3)  
RGT H 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON 42 deg C

STAGE (4)  
RCT K 149-45-1  
SOL 7732-18-5 Water

PRO O 491576-85-3

E3 ANSWER 3 OF 5 CASREACT COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 140:78500 CASREACT  
 TITLE: Synthesis of water-soluble near-infrared cyanine dyes functionalized with [(succinimido)oxy]carbonyl group  
 AUTHOR(S): Strekowski, Lucjan; Mason, Christian J.; Lee, Hyeran; Gupta, Rajni; Sowell, John; Patonay, Gabor  
 CORPORATE SOURCE: Department of Chemistry, Georgia State University, Atlanta, GA, 30303, USA  
 SOURCE: Journal of Heterocyclic Chemistry (2003), 40(5), 913-916  
 CODEN: JHTCAD; ISSN: 0022-152X  
 PUBLISHER: HeteroCorporation  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB Two heptamethine cyanine dyes I (R1 = R2 = H; R1R2 = (CH:CH)2) suitable for labeling of biomols. at a primary amino group with a near-IR chromophore/fluorophore ( $\lambda_{max}/\lambda_{em}$  = 800/830 nm and 837/864 nm) have been synthesized from readily available starting materials. Despite the high mol. complexity of intermediate and final products, all these compds. have been obtained in an anal. pure form by using crystallization only.  
 REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE  
 FORMAT

RX(7) OF 13 COMPOSED OF RX(1), RX(3)  
 RX(7) 2 A + B + G ==> K

L3 ANSWER 3 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)  
 RX(1) RCT A 63666-10-4, B 63857-00-1  
 RGT D 127-09-3 AcONa  
 PRO C 640279-12-5  
 SOL 64-17-5 EtOH  
 NTE stereoselective

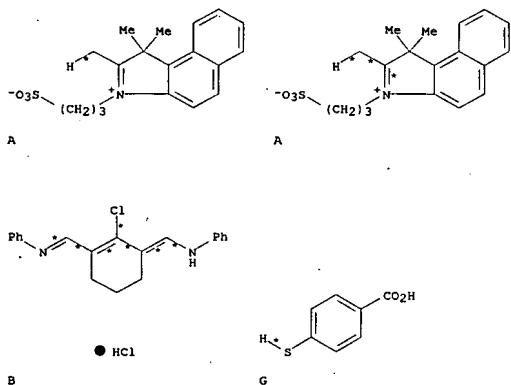
RX(3) RCT C 640279-12-5, G 1074-36-8

STAGE(1)  
 SOL 68-12-2 DMF  
 CON 24 hours, 23 deg C

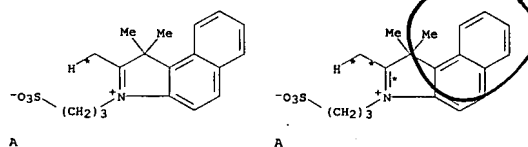
STAGE(2)  
 SOL 64-17-5 EtOH, 60-29-7 Et2O

PRO K 367251-79-4

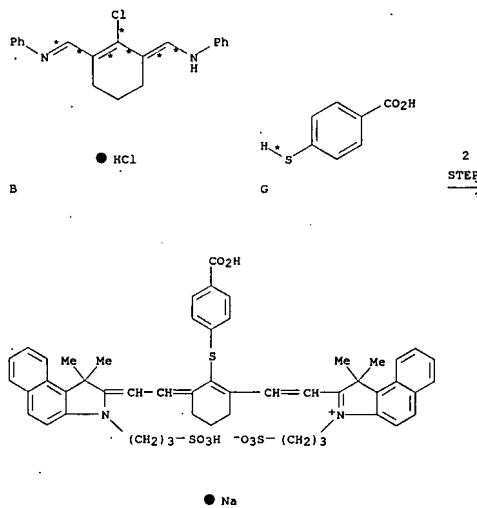
RX(11) OF 13 COMPOSED OF RX(1), RX(3), RX(5)  
 RX(11) 2 A + B + G + L ==> N



L3 ANSWER 3 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

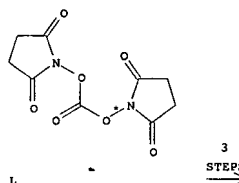


Not  
claimed



K  
 YIELD 90%

L3 ANSWER 3 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*  
 PAGE 2-A

N  
 YIELD 88%

RX(1) RCT A 63666-10-4, B 63857-00-1  
 RGT D 127-09-3 AcONa  
 PRO C 640279-12-5  
 SOL 64-17-5 EtOH  
 NTE stereoselective

RX(3) RCT C 640279-12-5, G 1074-36-8

STAGE(1)  
 SOL 68-12-2 DMF  
 CON 24 hours, 23 deg C

STAGE(2)  
 SOL 64-17-5 EtOH, 60-29-7 Et2O

PRO K 367251-79-4

RX(5) RCT K 367251-79-4, L 74124-79-1

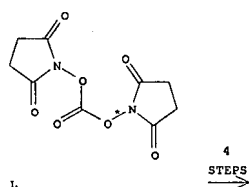
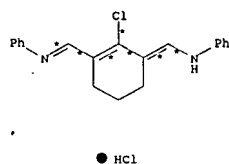
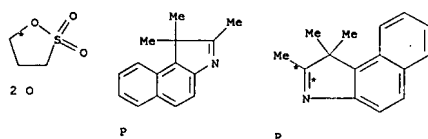
STAGE(1)  
 SOL 68-12-2 DMF  
 CON 24 hours, 23 deg C

STAGE(2)  
 SOL 60-29-7 Et2O  
 CON 30 minutes, 23 deg C

PRO N 367251-80-7

RX(12) OF 13 COMPOSED OF RX(6), RX(1), RX(3), RX(5)

L3 ANSWER 3 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)  
RX(12) 2 O + 2 P + B + G + L ==> N



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

L3 ANSWER 3 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

PAGE 2-A

● Na  
N  
YIELD 88%

RX(6) RCT O 1120-71-4, P 41532-84-7  
PRO A 63666-10-4  
NTE no exptl. detail

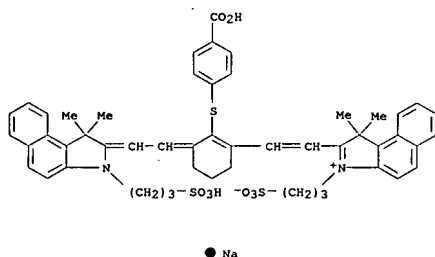
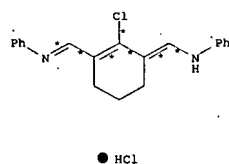
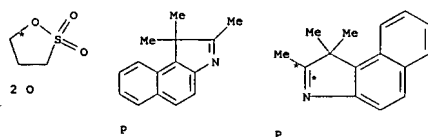
RX(1) RCT A 63666-10-4, B 63857-00-1  
RGT D 127-09-3 AcONa  
PRO C 640279-12-5  
SOL 64-17-5 EtOH  
NTE stereoselective

RX(3) RCT C 640279-12-5, G 1074-36-8  
STAGE(1)  
SOL 68-12-2 DMF  
CON 24 hours, 23 deg C  
STAGE(2)  
SOL 64-17-5 EtOH, 60-29-7 Et2O  
PRO K 367251-79-4

RX(5) RCT K 367251-79-4, L 74124-79-1  
STAGE(1)  
SOL 68-12-2 DMF  
CON 24 hours, 23 deg C  
STAGE(2)  
SOL 60-29-7 Et2O  
CON 30 minutes, 23 deg C  
PRO N 367251-80-7

RX(13) OF 13 COMPOSED OF RX(6), RX(1), RX(3)  
RX(13) 2 O + 2 P + B + G ==> K

L3 ANSWER 3 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



K  
YIELD 90%

RX(6) RCT O 1120-71-4, P 41532-84-7  
PRO A 63666-10-4  
NTE no exptl. detail

L3 ANSWER 3 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

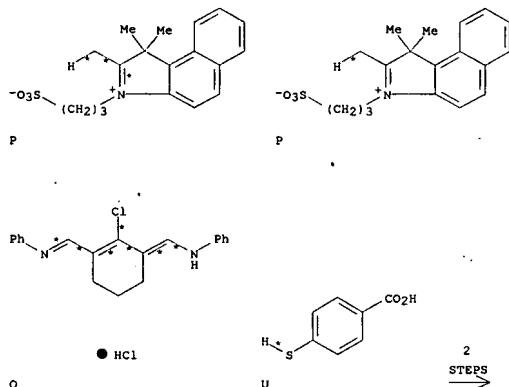
RX(1) RCT A 63666-10-4, B 63857-00-1  
RGT D 127-09-3 AcONa  
PRO C 640279-12-5  
SOL 64-17-5 EtOH  
NTE stereoselective

RX(3) RCT C 640279-12-5, G 1074-36-8  
STAGE(1)  
SOL 68-12-2 DMF  
CON 24 hours, 23 deg C  
STAGE(2)  
SOL 64-17-5 EtOH, 60-29-7 Et2O  
PRO K 367251-79-4

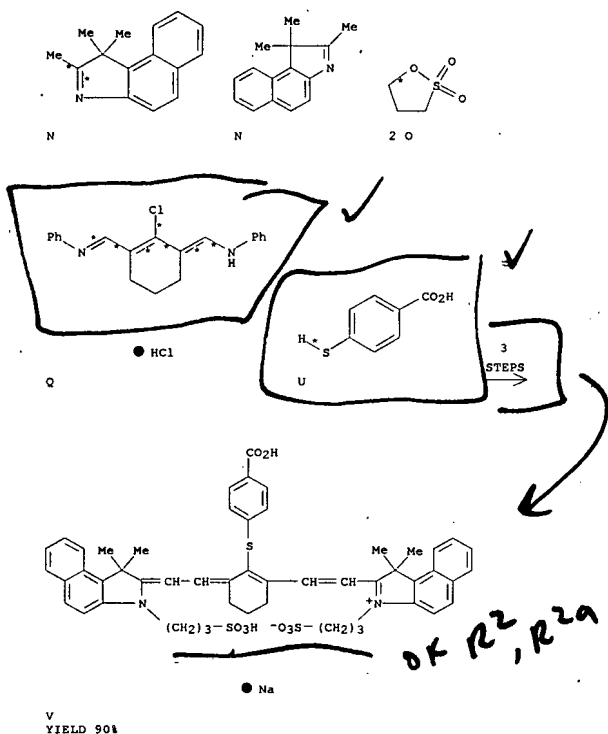


L3 ANSWER 4 OF 5 CASREACT COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 135:305176 CASREACT  
 TITLE: New heptamethine cyanine reagents for labeling of biomolecules with a near-infrared chromophore  
 AUTHOR(S): Strekowski, Lucjan; Gorecki, Tadeusz; Mason, J. Christian; Lee, Hyeran; Patonay, Gabor  
 CORPORATE SOURCE: Department of Chemistry, Georgia State University, Atlanta, GA, 30303, USA  
 SOURCE: Heterocyclic Communications (2001), 7(2), 117-122  
 CODEN: HCOMEX; ISSN: 0793-0283  
 PUBLISHER: Freund Publishing House Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The syntheses of two fluorescent cyanine dyes ( $\lambda_{\text{max}}$  = 1033 and 1060 nm in MeOH) with an isothiocyanato function and a succinimidoxycarbonyl-functionalized cyanine dye ( $\lambda_{\text{max}}$  = 837 nm in MeOH) for labeling of biomols. at amino groups are described.  
 REFERENCE COUNT: 8  
 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE  
 FORMAT

RX(10) OF 14 COMPOSED OF RX(5), RX(6)  
 RX(10) 2 P + Q + U ==> V

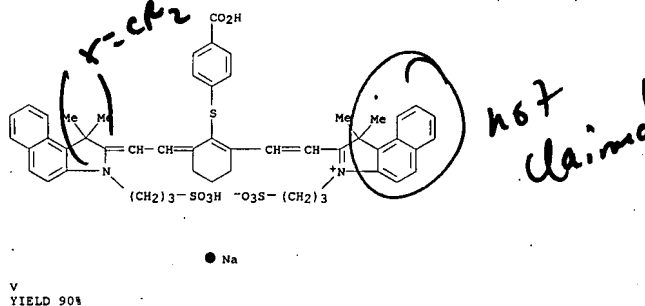


L3 ANSWER 4 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



RX(4) RCT N 41532-84-7, O 1120-71-4  
 PRO P 63666-10-4  
 NTE literature prepn.

L3 ANSWER 4 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



RX(5) RCT P 63666-10-4, Q 63857-00-1

STAGE(1)  
 RGT S 127-09-3 AcONa  
 SOL 64-17-5 EtOH

STAGE(2)  
 SOL 60-29-7 Et2O

PRO R 259261-66-0

RX(6) RCT R 259261-66-0, U 1074-36-8

STAGE(1)  
 SOL 68-12-2 DMF

STAGE(2)  
 SOL 60-29-7 Et2O

PRO V 367251-79-4

RX(12) OF 14 COMPOSED OF RX(4), RX(5), RX(6)  
 RX(12) 2 N + 2 O + Q + U ==> V

L3 ANSWER 4 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

RX(5) RCT P 63666-10-4, Q 63857-00-1

STAGE(1)  
 RGT S 127-09-3 AcONa  
 SOL 64-17-5 EtOH

STAGE(2)  
 SOL 60-29-7 Et2O

PRO R 259261-66-0

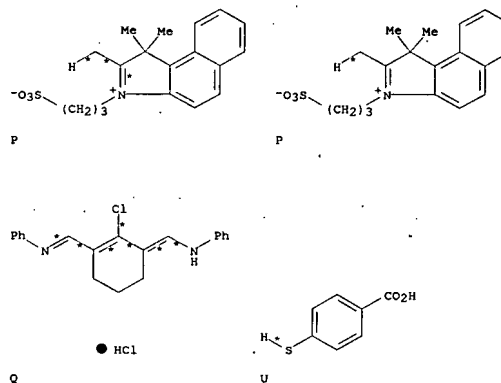
RX(6) RCT R 259261-66-0, U 1074-36-8

STAGE(1)  
 SOL 68-12-2 DMF

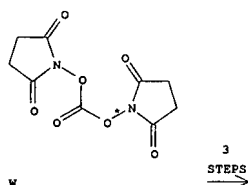
STAGE(2)  
 SOL 60-29-7 Et2O

PRO V 367251-79-4

RX(13) OF 14 COMPOSED OF RX(5), RX(6), RX(7)  
 RX(13) 2 P + Q + U + W ==> X



L3 ANSWER 4 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

PAGE 2-A

● Na

X  
YIELD 91%

RX(5) RCT P 63666-10-4, Q 63857-00-1

STAGE(1)  
RGT S 127-09-3 ACoNa  
SOL 64-17-5 EtOH

STAGE(2)  
SOL 60-29-7 Et2O

PRO R 259261-66-0

RX(6) RCT R 259261-66-0, U 1074-36-8

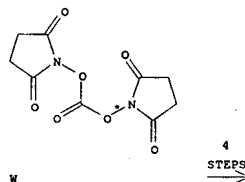
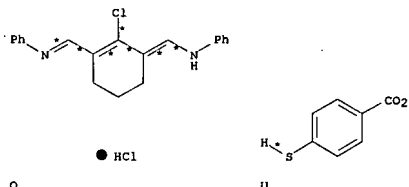
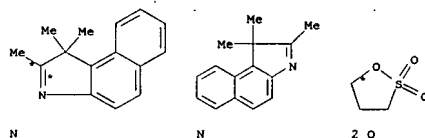
STAGE(1)  
SOL 68-12-2 DMF

STAGE(2)  
SOL 60-29-7 Et2O

PRO V 367251-79-4

RX(7) RCT V 367251-79-4, W 74124-79-1  
PRO X 367251-80-7  
SOL 68-12-2 DMF  
NTE literature prepn.

L3 ANSWER 4 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)  
RX(14) OF 14 COMPOSED OF RX(4), RX(5), RX(6), RX(7)  
RX(14) 2 N + 2 O + Q + U + W ==> X



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

L3 ANSWER 4 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

PAGE 2-A

● Na

X  
YIELD 91%

RX(4) RCT N 41532-84-7, O 1120-71-4  
PRO P 63666-10-4  
NTE literature prepn.

RX(5) RCT P 63666-10-4, Q 63857-00-1

STAGE(1)  
RGT S 127-09-3 ACoNa  
SOL 64-17-5 EtOH

STAGE(2)  
SOL 60-29-7 Et2O

PRO R 259261-66-0

RX(6) RCT R 259261-66-0, U 1074-36-8

STAGE(1)  
SOL 68-12-2 DMF

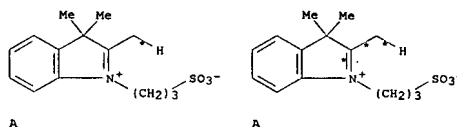
STAGE(2)  
SOL 60-29-7 Et2O

PRO V 367251-79-4

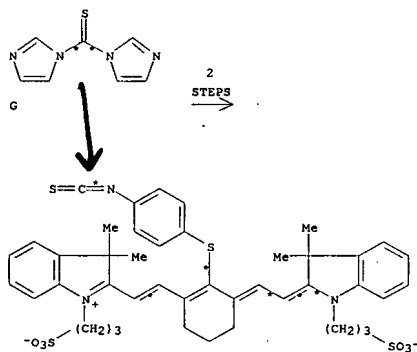
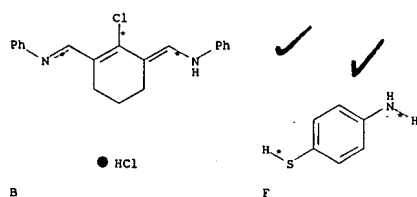
RX(7) RCT V 367251-79-4, W 74124-79-1  
PRO X 367251-80-7  
SOL 68-12-2 DMF  
NTE literature prepn.

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 127:231448 CASREACT  
TITLE: Functionalized Tricarbocyanine Dyes as Near-Infrared Fluorescent Probes for Biomolecules  
AUTHOR(S): Flanagan, James H., Jr.; Khan, Shaheer H.; Menchen, Steve; Soper, Steven A.; Hammer, Robert P.  
CORPORATE SOURCE: Department of Chemistry, Louisiana State University, Baton Rouge, LA, 70803-1804, USA  
SOURCE: Bioconjugate Chemistry (1997), 8(5), 751-756  
CODEN: BCCHES; ISSN: 1043-1802  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The syntheses of 3 novel functionalized tricarbocyanine dyes are described. These dyes containing isothiocyanate and succinimidyl ester functional groups are reactive toward primary amines and can be used as fluorescent probes for biol. pertinent compds. such as amino acids and functionalized dideoxynucleotides. The absorption and fluorescence maxima occur in the near-IR region of the spectrum (770-820 nm). The succinimidyl ester proved to be very sensitive to hydrolysis and was generated in situ to label amino acids and alkyl amines. The isothiocyanates were less susceptible to hydrolysis and were conjugated using organic modified [(40% (volume/volume) acetonitrile) buffers to amino acids. A dye with an alkyl isothiocyanate moiety showed conjugation to amino-functionalized dideoxynucleotide triphosphates.  
REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE  
FORMAT

RX(11) OF 44 COMPOSED OF RX(1), RX(2)  
RX(11) 2 A + B + F + G ==> H



L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

H  
YIELD 29%

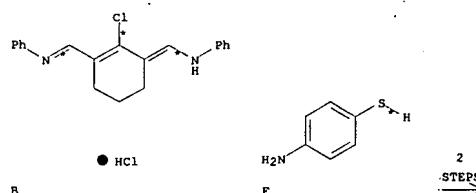
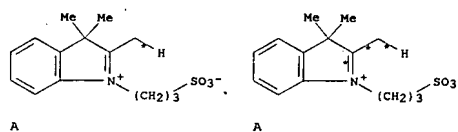
RX(1) RCT A 29636-96-2, B 195382-10-6  
 RGT D 127-09-3 AcONa  
 PRO C 160846-41-3  
 SOL 64-17-5 EtOH

RX(2) RCT F 1193-02-8, C 160846-41-3

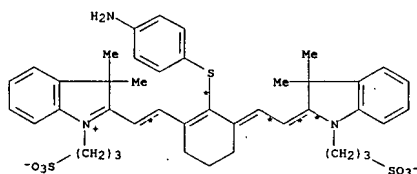
L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

STAGE(1)  
 SOL 68-12-2 DMF  
 STAGE(2)  
 RCT G 6160-65-2  
 STAGE(3)  
 SOL 60-29-7 Et2O  
 STAGE(4)  
 SOL 7732-18-5 Water, 67-56-1 MeOH  
 PRO H 160846-42-4

RX(12) OF 44 COMPOSED OF RX(1), RX(6)  
 RX(12) 2 A + B + F ==> X



L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

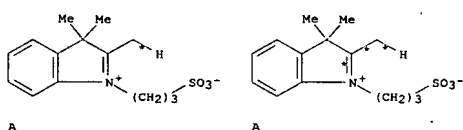
X  
YIELD 50%

RX(1) RCT A 29636-96-2, B 195382-10-6  
 RGT D 127-09-3 AcONa  
 PRO C 160846-41-3  
 SOL 64-17-5 EtOH

RX(6) RCT F 1193-02-8

STAGE(1)  
 SOL 68-12-2 DMF  
 STAGE(2)  
 RCT C 160846-41-3  
 PRO X 195382-11-7

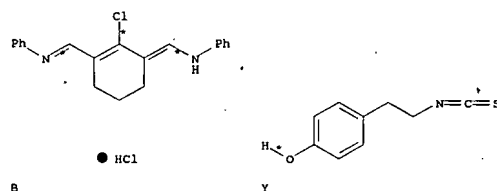
RX(13) OF 44 COMPOSED OF RX(1), RX(7)  
 RX(13) 2 A + B + Y ==> Z



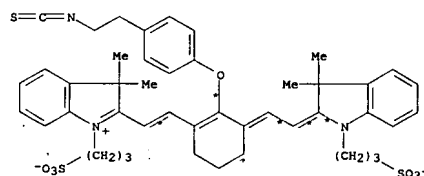
A

A

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



2  
 STEPS

Z  
YIELD 32%

RX(1) RCT A 29636-96-2, B 195382-10-6  
 RGT D 127-09-3 AcONa  
 PRO C 160846-41-3  
 SOL 64-17-5 EtOH

oRX(7) RCT Y 60114-04-7

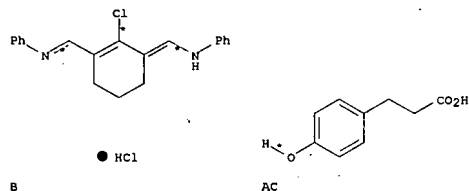
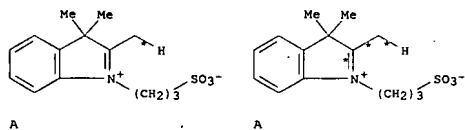
STAGE(1)  
 RGT AA 7646-69-7 NaH  
 SOL 68-12-2 DMF

STAGE(2)  
 RCT C 160846-41-3  
 SOL 68-12-2 DMF

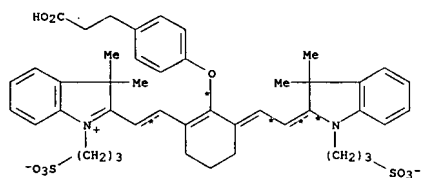
PRO Z 195382-08-2

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN  
 RX(14) OF 44 COMPOSED OF RX(1), RX(9)  
 RX(14) 2 A + B + AC ==> M

(Continued)



2  
STEPS

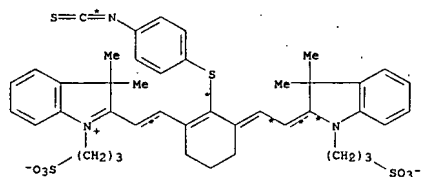


YIELD 31%

RX(1) RCT A 29636-96-2, B 195382-10-6  
 RGT D 127-09-3 AcONa  
 PRO C 160846-41-3  
 SOL 64-17-5 EtOH

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN

(Continued)



YIELD 39%

RX(1) RCT A 29636-96-2, B 195382-10-6  
 RGT D 127-09-3 AcONa  
 PRO C 160846-41-3  
 SOL 64-17-5 EtOH

RX(6) RCT F 1193-02-8

STAGE(1)  
 SOL 68-12-2 DMF

STAGE(2)  
 RCT C 160846-41-3

PRO X 195382-11-7

RX(10) RCT X 195382-11-7

STAGE(1)  
 RGT AE 497-19-8 Na2CO3  
 SOL 68-12-2 DMF

STAGE(2)  
 RCT AD 463-71-8

PRO H 160846-42-4

RX(21) OF 44 COMPOSED OF REACTION SEQUENCE RX(8), RX(7)  
 AND REACTION SEQUENCE RX(1), RX(7)

...AB + G ==> Y...  
 ...2 A + B + Y ==> Z

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN

(Continued)

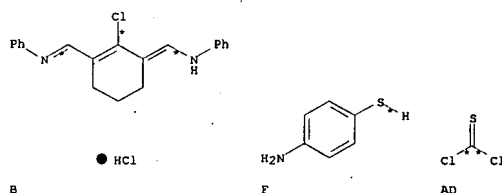
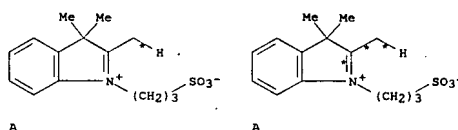
RX(9) RCT AC 501-97-3

STAGE(1)  
 RGT AA 7646-69-7 NaH  
 SOL 68-12-2 DMF

STAGE(2)  
 RCT C 160846-41-3

PRO M 195382-12-8

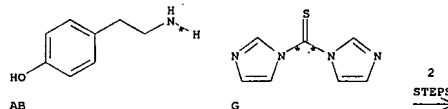
RX(20) OF 44 COMPOSED OF RX(1), RX(6), RX(10)  
 RX(20) 2 A + B + F + AD ==> H



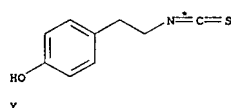
3  
STEPS

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN

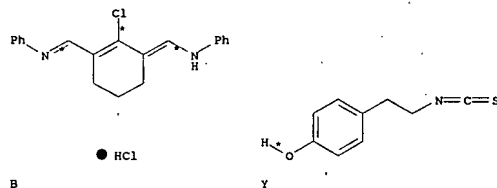
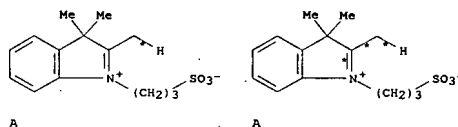
(Continued)



2  
STEPS



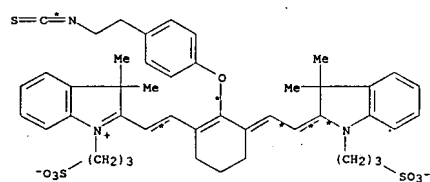
START NEXT REACTION SEQUENCE



2  
STEPS

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN

(Continued)

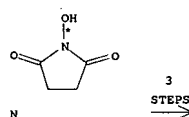
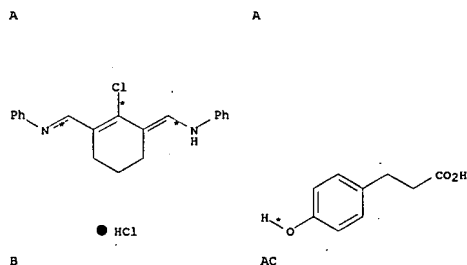
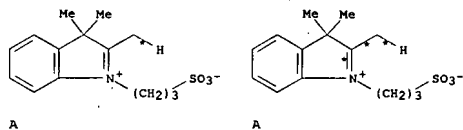


Z  
YIELD 32%

RX(8) RCT AB 51-67-2  
STAGE(1)  
SOL 68-12-2 DMF  
STAGE(2)  
RCT G 6160-65-2  
PRO Y 60114-04-7  
RX(1) RCT A 29636-96-2, B 195382-10-6  
RGT D 127-09-3 AcONa  
PRO C 160846-41-3  
SOL 64-17-5 EtOH  
RX(7) RCT Y 60114-04-7  
STAGE(1)  
RGT AA 7646-69-7 NaH  
SOL 68-12-2 DMF  
STAGE(2)  
RCT C 160846-41-3  
SOL 68-12-2 DMF  
PRO Z 195382-08-2

RX(22) OF 44 COMPOSED OF RX(1), RX(9), RX(3)  
RX(22) 2 A + B + AC + N ==> O

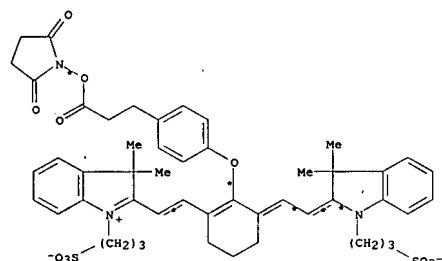
L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



3  
STEPS

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN

(Continued)

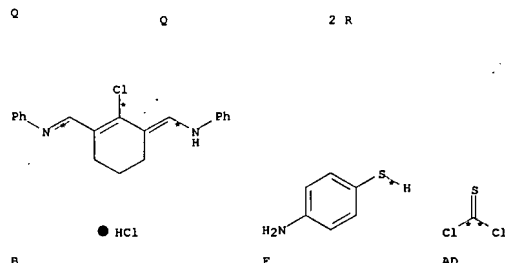
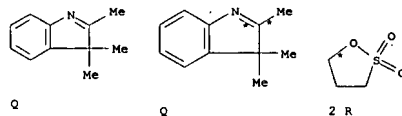


O

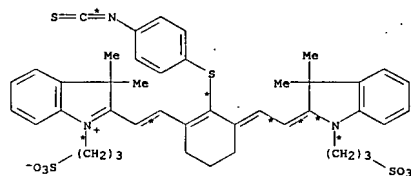
RX(1) RCT A 29636-96-2, B 195382-10-6  
RGT D 127-09-3 AcONa  
PRO C 160846-41-3  
SOL 64-17-5 EtOH  
RX(9) RCT AC 501-97-3  
STAGE(1)  
RGT AA 7646-69-7 NaH  
SOL 68-12-2 DMF  
STAGE(2)  
RCT C 160846-41-3  
PRO M 195382-12-8  
RX(3) RCT M 195382-12-8, N 6066-82-6  
STAGE(1)  
SOL 68-12-2 DMF  
STAGE(2)  
RGT P 538-75-0 DCC  
PRO O 195382-09-3

RX(23) OF 44 COMPOSED OF RX(4), RX(1), RX(6), RX(10)  
RX(23) 2 Q + 2 R + B + F + AD ==> H

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



4  
STEPS



H  
YIELD 39%

RX(4) RCT Q 1640-39-7, R 1120-71-4  
PRO A 29636-96-2  
SOL 108-88-3 PhMe  
RX(1) RCT A 29636-96-2, B 195382-10-6

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

RGT D 127-09-3 AcONa  
PRO C 160846-41-3  
SOL 64-17-5 EtOH

RX(6) RCT F 1193-02-8

STAGE(1)  
SOL 68-12-2 DMF

STAGE(2)  
RCT C 160846-41-3

PRO X 195382-11-7

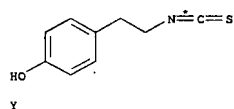
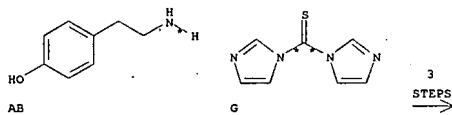
RX(10) RCT X 195382-11-7

STAGE(1)  
RGT AE 497-19-8 Na2CO3  
SOL 68-12-2 DMF

STAGE(2)  
RCT AD 463-71-8

PRO H 160846-42-4

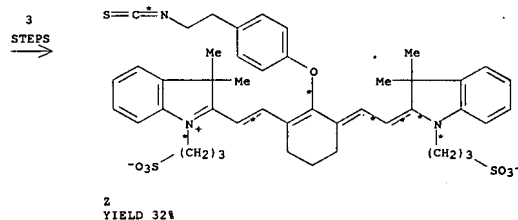
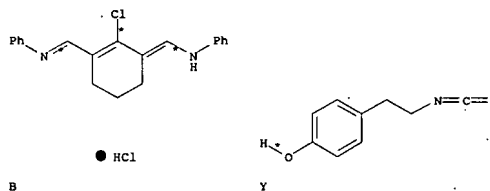
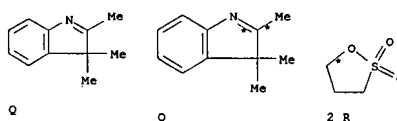
RX(24) OF 44 COMPOSED OF REACTION SEQUENCE RX(8), RX(7)  
AND REACTION SEQUENCE RX(4), RX(1), RX(7)  
...AB + G ==> Y...  
...2 Q + 2 R + B + Y ==> Z



START NEXT REACTION SEQUENCE

2

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



RX(8) RCT AB 51-67-2

STAGE(1)  
SOL 68-12-2 DMF

STAGE(2)  
RCT G 6160-65-2

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

PRO Y 60114-04-7

RX(4) RCT Q 1640-39-7, R 1120-71-4  
PRO A 29636-96-2  
SOL 108-88-3 PhMe

RX(1) RCT A 29636-96-2, B 195382-10-6  
RGT D 127-09-3 AcONa  
PRO C 160846-41-3  
SOL 64-17-5 EtOH

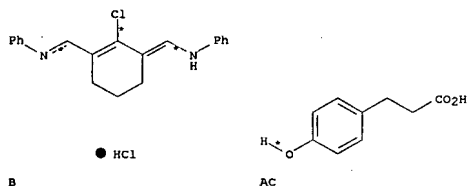
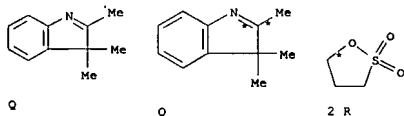
RX(7) RCT Y 60114-04-7

STAGE(1)  
RGT AA 7646-69-7 NaH  
SOL 68-12-2 DMF

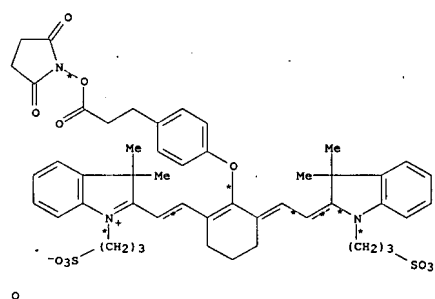
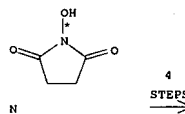
STAGE(2)  
RCT C 160846-41-3  
SOL 68-12-2 DMF

PRO Z 195382-08-2

RX(25) OF 44 COMPOSED OF RX(4), RX(1), RX(9), RX(3)  
RX(25) 2 Q + 2 R + B + AC + N ==> O



L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



RX(4) RCT Q 1640-39-7, R 1120-71-4  
PRO A 29636-96-2  
SOL 108-88-3 PhMe

RX(1) RCT A 29636-96-2, B 195382-10-6  
RGT D 127-09-3 AcONa  
PRO C 160846-41-3  
SOL 64-17-5 EtOH

RX(9) RCT AC 501-97-3

STAGE(1)  
RGT AA 7646-69-7 NaH  
SOL 68-12-2 DMF

STAGE(2)  
RCT C 160846-41-3

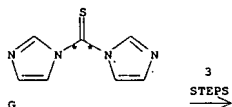
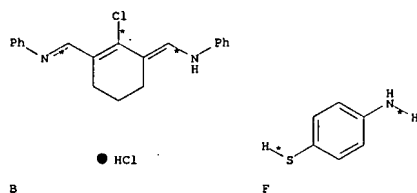
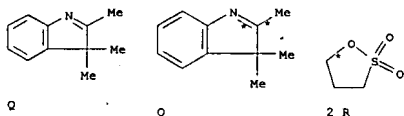
PRO M 195382-12-8

RX(3) RCT M 195382-12-8, N 6066-82-6

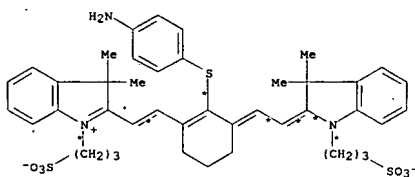
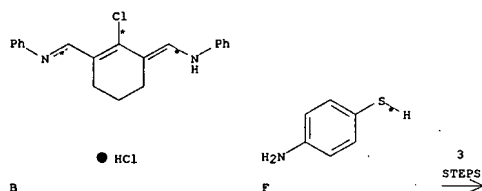
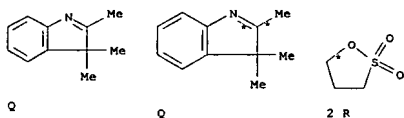
L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

STAGE(1)  
SOL 68-12-2 DMFSTAGE(2)  
RGT P 538-75-0 DCC

PRO O 195382-09-3

RX(29) OF 44 COMPOSED OF RX(4), RX(1), RX(2)  
RX(29) 2 Q + 2 R + B + F + G ==> H

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

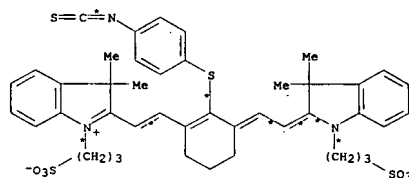


YIELD 50%

RX(4) RCT Q 1640-39-7, R 1120-71-4  
PRO A 29636-96-2  
SOL 108-88-3 PhMeRX(1) RCT A 29636-96-2, B 195382-10-6  
RGT D 127-09-3 AcONa  
PRO C 160846-41-3  
SOL 64-17-5 EtOH

RX(6) RCT F 1193-02-8

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



YIELD 29%

RX(4) RCT Q 1640-39-7, R 1120-71-4  
PRO A 29636-96-2  
SOL 108-88-3 PhMeRX(1) RCT A 29636-96-2, B 195382-10-6  
RGT D 127-09-3 AcONa  
PRO C 160846-41-3  
SOL 64-17-5 EtOH

RX(2) RCT F 1193-02-8, C 160846-41-3

STAGE(1)  
SOL 68-12-2 DMFSTAGE(2)  
RCT G 6160-65-2STAGE(3)  
SOL 60-29-7 Et2OSTAGE(4)  
SOL 7732-18-5 Water, 67-56-1 MeOH

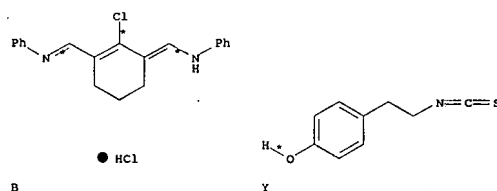
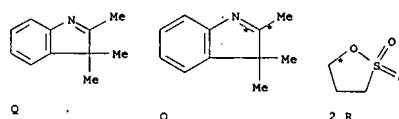
PRO H 160846-42-4

RX(30) OF 44 COMPOSED OF RX(4), RX(1), RX(6)  
RX(30) 2 Q + 2 R + B + F ==> X

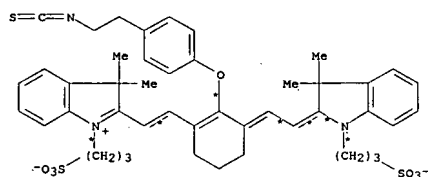
L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

STAGE(1)  
SOL 68-12-2 DMFSTAGE(2)  
RCT C 160846-41-3

PRO X 195382-11-7

RX(31) OF 44 COMPOSED OF RX(4), RX(1), RX(7)  
RX(31) 2 Q + 2 R + B + Y ==> Z

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

Z  
YIELD 32%

RX(4) RCT Q 1640-39-7, R 1120-71-4  
PRO A 29636-96-2  
SOL 108-88-3 PhMe

RX(1) RCT A 29636-96-2, B 195382-10-6  
RGT D 127-09-3 AcONa  
PRO C 160846-41-3  
SOL 64-17-5 EtOH

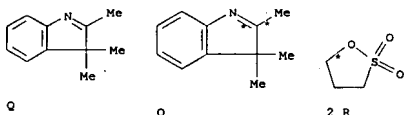
RX(7) RCT Y 60114-04-7

STAGE(1)  
RGT AA 7646-69-7 NaH  
SOL 68-12-2 DMF

STAGE(2)  
RCT C 160846-41-3  
SOL 68-12-2 DMF

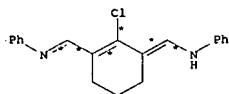
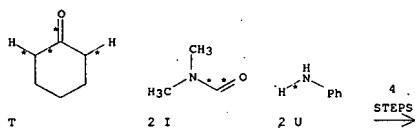
PRO Z 195382-08-2

RX(32) OF 44 COMPOSED OF RX(4), RX(1), RX(9)  
RX(32) 2 Q + 2 R + B + AC ==> M



L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

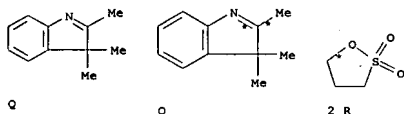
RX(38) OF 44 COMPOSED OF REACTION SEQUENCE RX(5), RX(1), RX(6), RX(10)  
AND REACTION SEQUENCE RX(4), RX(1), RX(6), RX(10)  
...T + 2 I + 2 U ==> B...  
...2 Q + 2 R + B + F + AD ==> H



● HCl

B

START NEXT REACTION SEQUENCE

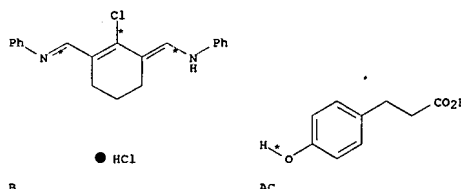
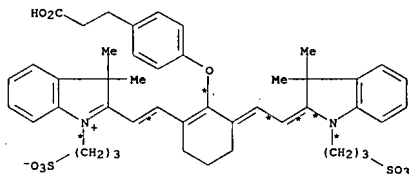


Q

Q

2 R

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

3  
STEPSM  
YIELD 31%

RX(4) RCT Q 1640-39-7, R 1120-71-4  
PRO A 29636-96-2  
SOL 108-88-3 PhMe

RX(1) RCT A 29636-96-2, B 195382-10-6  
RGT D 127-09-3 AcONa  
PRO C 160846-41-3  
SOL 64-17-5 EtOH

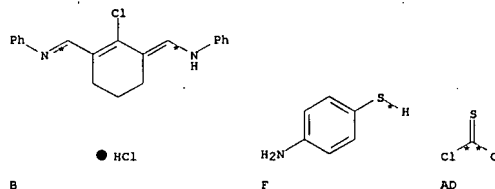
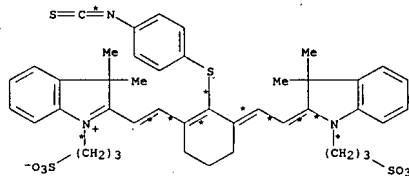
RX(9) RCT AC 501-97-3

STAGE(1)  
RGT AA 7646-69-7 NaH  
SOL 68-12-2 DMF

STAGE(2)  
RCT C 160846-41-3

PRO M 195382-12-8

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

4  
STEPSH  
YIELD 39%

RX(5) RCT T 108-94-1, I 68-12-2

STAGE(1)  
RGT V 10025-87-3 POCl3  
SOL 68-12-2 DMF

STAGE(2)  
RCT U 62-53-3  
SOL 64-17-5 EtOH

STAGE(3)  
RGT W 7647-01-0 HCl  
SOL 7732-18-5 Water

PRO B 195382-10-6

RX(4) RCT Q 1640-39-7, R 1120-71-4



L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)  
 PRO A 29636-96-2  
 SOL 108-88-3 PhMe

RX(1) RCT A 29636-96-2, B 195382-10-6  
 RGT D 127-09-3 AcONa  
 PRO C 160846-41-3  
 SOL 64-17-5 EtOH

RX(6) RCT F 1193-02-8  
 STAGE(1)  
 SOL 68-12-2 DMF  
 STAGE(2)  
 RCT C 160846-41-3

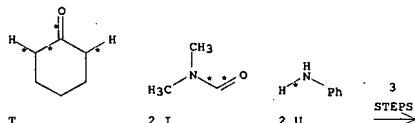
PRO X 195382-11-7

RX(10) RCT X 195382-11-7  
 STAGE(1)  
 RGT AE 497-19-8 Na2CO3  
 SOL 68-12-2 DMF

STAGE(2)  
 RCT AD 463-71-8

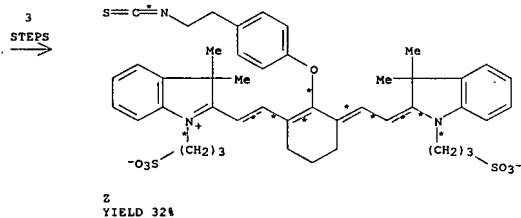
PRO H 160846-42-4

RX(39) OF 44 COMPOSED OF REACTION SEQUENCE RX(5), RX(1), RX(7)  
 AND REACTION SEQUENCE RX(8), RX(7)  
 AND REACTION SEQUENCE RX(4), RX(1), RX(7)  
 ...T + 2 I + 2 U ==> B...  
 ...AB + G ==> Y...  
 ...2 Q + 2 R + B + Y ==> Z



START NEXT REACTION SEQUENCE

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



RX(5) RCT T 108-94-1, I 68-12-2  
 STAGE(1)  
 RGT V 10025-87-3 POCl3  
 SOL 68-12-2 DMF

STAGE(2)  
 RCT U 62-53-3  
 SOL 64-17-5 EtOH

STAGE(3)  
 RGT W 7647-01-0 HCl  
 SOL 7732-18-5 Water

PRO B 195382-10-6

RX(8) RCT AB 51-67-2  
 STAGE(1)  
 SOL 68-12-2 DMF

STAGE(2)  
 RCT G 6160-65-2

PRO Y 60114-04-7

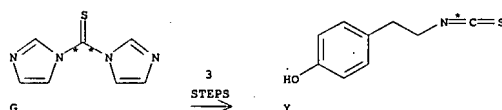
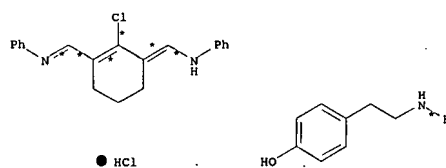
RX(4) RCT Q 1640-39-7, R 1120-71-4  
 PRO A 29636-96-2  
 SOL 108-88-3 PhMe

RX(1) RCT A 29636-96-2, B 195382-10-6  
 RGT D 127-09-3 AcONa  
 PRO C 160846-41-3  
 SOL 64-17-5 EtOH

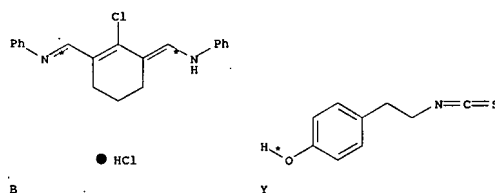
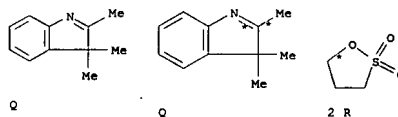
RX(7) RCT Y 60114-04-7

STAGE(1)  
 RGT AA 7646-69-7 NaH

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



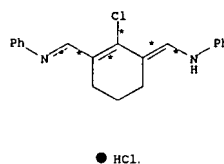
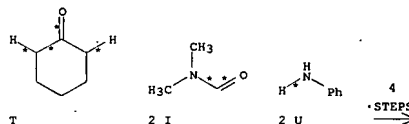
START NEXT REACTION SEQUENCE



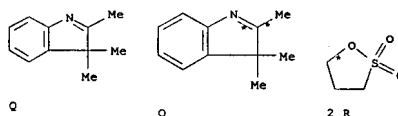
L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

STAGE(2)  
 RCT C 160846-41-3  
 SOL 68-12-2 DMF  
 PRO Z 195382-08-2

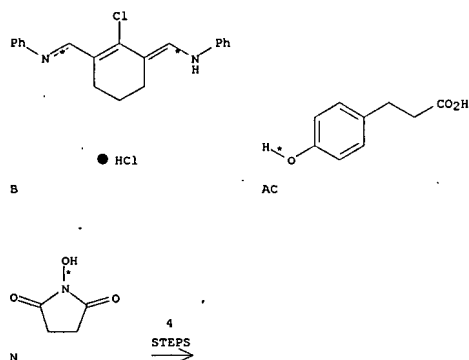
RX(40) OF 44 COMPOSED OF REACTION SEQUENCE RX(5), RX(1), RX(9), RX(3)  
 AND REACTION SEQUENCE RX(4), RX(1), RX(9), RX(3)  
 ...T + 2 I + 2 U ==> B...  
 ...2 Q + 2 R + B + AC + N ==> O



START NEXT REACTION SEQUENCE



L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(5) RCT T 108-94-1, I 68-12-2

STAGE(1)  
RGT V 10025-87-3 POCl3  
SOL 68-12-2 DMF

STAGE(2)  
RCT U 62-53-3  
SOL 64-17-5 EtOH

STAGE(3)  
RGT W 7647-01-0 HCl  
SOL 7732-18-5 Water

PRO B 195382-10-6

RX(4) RCT Q 1640-39-7, R 1120-71-4  
PRO A 29636-96-2  
SOL 108-88-3 PhMe

RX(1) RCT A 29636-96-2, B 195382-10-6  
RGT D 127-09-3 AcONa  
PRO C 160846-41-3

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

RX(9) RCT AC 501-97-3

STAGE(1)  
RGT AA 7646-69-7 NaH  
SOL 68-12-2 DMF

STAGE(2)  
RCT C 160846-41-3

PRO M 195382-12-8

RX(3) RCT M 195382-12-8, N 6066-82-6

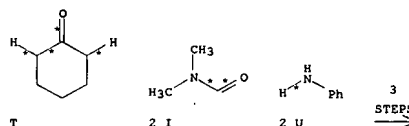
STAGE(1)  
SOL 68-12-2 DMF

STAGE(2)  
RGT P 538-75-0 DCC

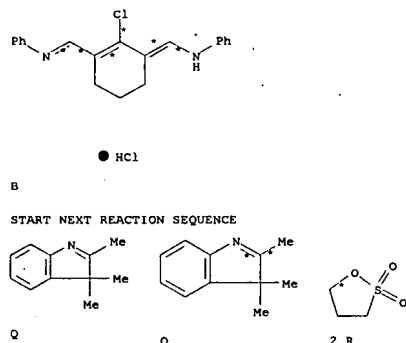
PRO O 195382-09-3

RX(41) OF 44 COMPOSED OF REACTION SEQUENCE RX(5), RX(1), RX(2)  
AND REACTION SEQUENCE RX(4), RX(1), RX(2)

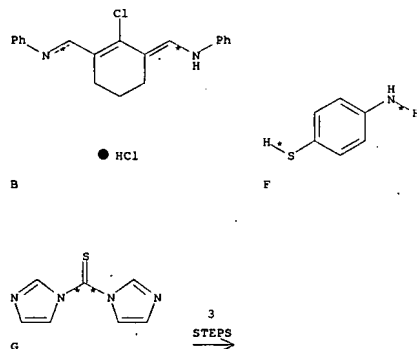
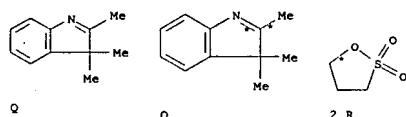
...T + 2 I + 2 U ==> B...  
...2 Q + 2 R + B + F + G ==> H



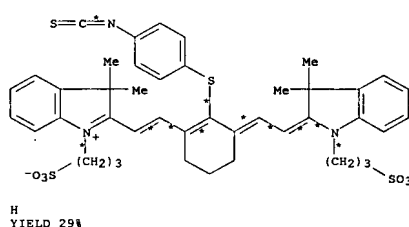
L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



START NEXT REACTION SEQUENCE



L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

H  
YIELD 29%

RX(5) RCT T 108-94-1, I 68-12-2

STAGE(1)  
RGT V 10025-87-3 POCl3  
SOL 68-12-2 DMF

STAGE(2)  
RCT U 62-53-3  
SOL 64-17-5 EtOH

STAGE(3)  
RGT W 7647-01-0 HCl  
SOL 7732-18-5 Water

PRO B 195382-10-6

RX(4) RCT Q 1640-39-7, R 1120-71-4  
PRO A 29636-96-2  
SOL 108-88-3 PhMe

RX(1) RCT A 29636-96-2, B 195382-10-6  
RGT D 127-09-3 AcONa  
PRO C 160846-41-3  
SOL 64-17-5 EtOH

RX(2) RCT F 1193-02-8, C 160846-41-3

STAGE(1)  
SOL 68-12-2 DMF

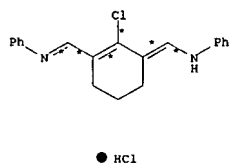
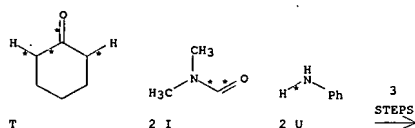
STAGE(2)  
RCT G 6160-65-2

STAGE(3)  
SOL 60-29-7 Et2O

STAGE(4)  
SOL 7732-18-5 Water, 67-56-1 MeOH

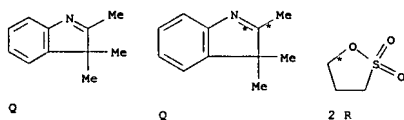
L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)  
PRO H 160846-42-4

RX(42) OF 44 COMPOSED OF REACTION SEQUENCE RX(5), RX(1), RX(6)  
AND REACTION SEQUENCE RX(4), RX(1), RX(6)  
...T + 2 I + 2 U ==> B...  
...2 Q + 2 R + B + F ==> X



B

START NEXT REACTION SEQUENCE



Q

Q

2 R

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

RX(1)      RCT A 29636-96-2, B 195382-10-6  
RGT D 127-09-3 AcONa  
PRO C 160846-41-3  
SOL 64-17-5 EtOH

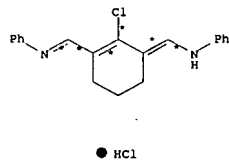
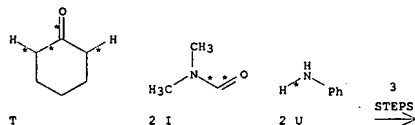
RX(6)      RCT F 1193-02-8

STAGE(1)  
SOL 68-12-2 DMF

STAGE(2)  
RCT C 160846-41-3

PRO X 195382-11-7

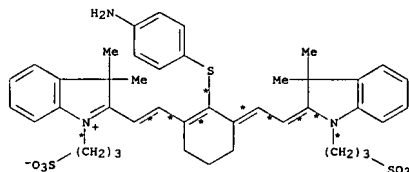
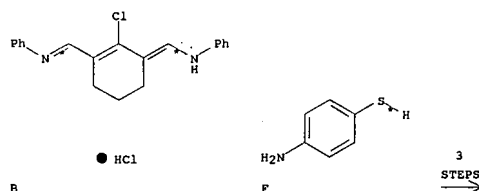
RX(43) OF 44 COMPOSED OF REACTION SEQUENCE RX(5), RX(1), RX(7)  
AND REACTION SEQUENCE RX(4), RX(1), RX(7)  
...T + 2 I + 2 U ==> B...  
...2 Q + 2 R + B + Y ==> Z



B

START NEXT REACTION SEQUENCE

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



X  
YIELD 50%

RX(5)      RCT T 108-94-1, I 68-12-2

STAGE(1)  
RGT V 10025-87-3 POC13  
SOL 68-12-2 DMF

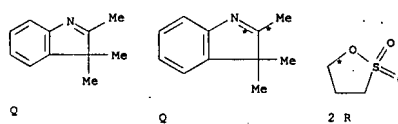
STAGE(2)  
RCT U 62-53-3  
SOL 64-17-5 EtOH

STAGE(3)  
RGT W 7647-01-0 HCl  
SOL 7732-18-5 Water

PRO B 195382-10-6

RX(4)      RCT Q 1640-39-7, R 1120-71-4  
PRO A 29636-96-2  
SOL 108-88-3 PhMe

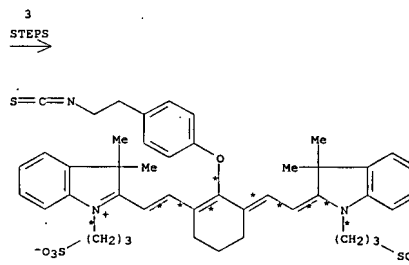
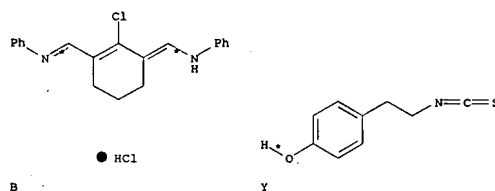
L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



Q

Q

2 R



Z  
YIELD 32%

RX(5)      RCT T 108-94-1, I 68-12-2

STAGE(1)  
RGT V 10025-87-3 POC13  
SOL 68-12-2 DMF

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

STAGE(2)  
 RCT U 62-53-3  
 SOL 64-17-5 EtOH

STAGE(3)  
 RGT W 7647-01-0 HCl  
 SOL 7732-18-5 Water

PRO B 195382-10-6

RX(4) RCT Q 1640-39-7, R 1120-71-4  
 PRO A 29636-96-2  
 SOL 108-88-3 PhMe

RX(1) RCT A 29636-96-2, B 195382-10-6  
 RGT D 127-09-3 AcONa  
 PRO C 160846-41-3  
 SOL 64-17-5 EtOH

RX(7) RCT Y 60114-04-7

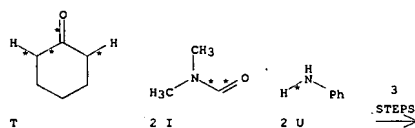
STAGE(1)  
 RGT AA 7646-69-7 NaH  
 SOL 68-12-2 DMF

STAGE(2)  
 RCT C 160846-41-3  
 SOL 68-12-2 DMF

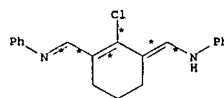
PRO Z 195382-08-2

RX(44) OF 44 COMPOSED OF REACTION SEQUENCE RX(5), RX(1), RX(9)  
 AND REACTION SEQUENCE RX(4), RX(1), RX(9)

...T + 2 I + 2 U ==> B...  
 ...2 Q + 2 R + B + AC ==> H



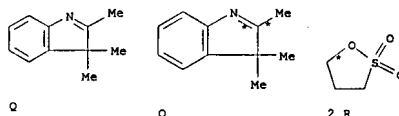
L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



● HCl

B

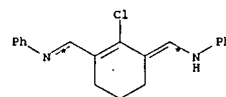
START NEXT REACTION SEQUENCE



Q

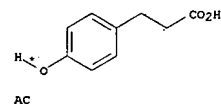
Q

2 R



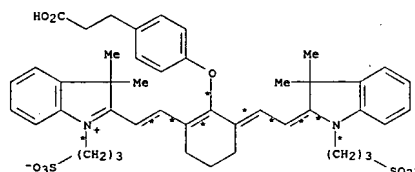
● HCl

B



3  
STEPS

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



M  
 YIELD 31%

RX(5) RCT T 108-94-1, I 68-12-2

STAGE(1)  
 RGT V 10025-87-3 POCl3  
 SOL 68-12-2 DMF

STAGE(2)  
 RCT U 62-53-3  
 SOL 64-17-5 EtOH

STAGE(3)  
 RGT W 7647-01-0 HCl  
 SOL 7732-18-5 Water

PRO B 195382-10-6

RX(4) RCT Q 1640-39-7, R 1120-71-4  
 PRO A 29636-96-2  
 SOL 108-88-3 PhMe

RX(1) RCT A 29636-96-2, B 195382-10-6  
 RGT D 127-09-3 AcONa  
 PRO C 160846-41-3  
 SOL 64-17-5 EtOH

RX(9) RCT AC 501-97-3

STAGE(1)  
 RGT AA 7646-69-7 NaH  
 SOL 68-12-2 DMF

STAGE(2)  
 RCT C 160846-41-3

PRO M 195382-12-8